

## **APPENDIX B**

# **INTEGRATING EXTERNAL MODELS OR MEASURED DATA INTO TRIM.FaTE**

[This page intentionally left blank.]

## **APPENDIX B**

# **INTEGRATING EXTERNAL MODELS OR MEASURED DATA INTO TRIM.FaTE**

At some point, it may be desirable to use either measured data or the output of other models with the TRIM.FaTE model. In either case, there are two basic forms that the data can take: (1) fluxes into certain compartments (*e.g.*, deposition rates), or (2) calculated/specified concentrations or chemical mass in certain compartments. The first case is the simpler of the two, as it requires only adding additional source terms to the affected compartments. The second case has more of an impact on the system of equations used in the modeling, and is the focus of this Appendix.

### **B.1 COMPROMISES THAT MUST BE MADE IN ORDER TO USE EXTERNALLY DERIVED COMPARTMENT CONCENTRATIONS**

The incorporation of externally derived compartment concentrations into *any* multimedia model dictates that compromises be made with regard to preserving chemical mass balance. The basic problem is the loss of chemical mass from the compartments that send a chemical to the compartment for which an externally derived compartment concentration is used. Since the receiving compartment will not receive the chemical, it is effectively lost from the system. The only way to avoid this loss of chemical mass is to modify all of the links to the “constant” compartments so that this exchange does not take place (*e.g.*, disable resuspension from surface soil to the air domain if the results of an air model are to be used).

While we will know mathematically how much mass has been lost through these processes, the chemical lost will not be allowed to participate in any further exchanges with other compartments. Whether this is acceptable or not depends on the attitude of the user, but this compromise is unavoidable if they are to use externally derived compartment concentrations.

### **B.2 IMPLEMENTATION DETAILS IN THE CASE OF FIRST-ORDER TRANSFERS – CASE OF CONSTANT INPUTS**

In this section, explicit details are provided for incorporating externally derived compartment concentrations for selected compartments in the case where these concentrations are constant for the time period of interest. The general case where the values from externally derived compartment concentrations change with time can be addressed by sequentially using this method over the different intervals over which the values from the externally derived compartment concentrations are constant.

For a given time interval in which the parameters are constant with time, the system of differential equations to be solved is:

$$\frac{d\vec{N}}{dt} = A \vec{N} + \vec{s} \quad (1)$$

where  $\vec{N}$  is the vector of the mass of chemical(s) in each compartment, given by:

$$\vec{N} = \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} \quad (2)$$

where  $n_i(t)$  is the mass of a particular chemical in a compartment/chemical pair,  $m$  is the total number of compartment/chemical pairs;  $A$  is the matrix of transfer factors describing transport between compartment/chemical pairs:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \quad (3)$$

and  $\vec{s}$  is the vector of sources terms for each chemical in each compartment.

The fact that chemical mass balance is preserved implies that the matrix  $A$  satisfies two basic conditions:

$$a_{ij} \neq 0, \text{ if } i \neq j \text{ and } a_{ii} \neq 0 \quad (4)$$

$$a_{jj} = - \sum_{i=1, i \neq j}^m a_{ij} \quad (5)$$

Using externally derived compartment concentrations is equivalent to fixing the concentration/chemical mass in some compartments. This can be done by solving a reduced system of differential equations, using constant values for the applicable terms  $n_i(t)$ . This can be conceptualized as using “virtual sources” for the relevant compartment/chemical pairs, with each (time-dependent) virtual source set so that the mass of chemical is constant.

For example, if there is only one chemical being considered, and we want the concentration/mass to be fixed in the first compartment, say  $n_1(t) = M_1$ , then  $dn_1/dt = 0$ , and the original system becomes:

$$\frac{d}{dt} \begin{bmatrix} M_1 \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} M_1 \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{bmatrix} \quad (6)$$

Since the derivative of a constant is zero, examining the first row of the above system shows that:

$$0 = \sum_{i=1}^m n_i(t) a_{1i} + s_1(t) \quad (7)$$

*i.e.*, the virtual source  $s_1(t)$  in the first compartment is given by:

$$\begin{aligned} s_1(t) &= -\sum_{i=1}^m n_i(t) a_{1i} \\ &= -Ma_{11} - \sum_{i=2}^m n_i(t) a_{1i} \end{aligned} \quad (8)$$

The terms  $n_i(t)$  for  $i > 1$  can be determined by solving the system of differential equations obtained by eliminating the first row, and using  $n_1(t) = M$ :

$$\begin{aligned} \frac{d}{dt} \begin{bmatrix} n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} &= \begin{bmatrix} a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} M \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_2 \\ \vdots \\ s_m \end{bmatrix} \\ &= \begin{bmatrix} a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & \\ a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_2 + Ma_{21} \\ \vdots \\ s_m + Ma_{m1} \end{bmatrix} \end{aligned} \quad (9)$$

This system of differential equations is of the same form as the original equation, and can be solved using the same solver used for the original equation. However, it can also be rewritten as a system of the same size as the original system by adding the differential equation  $dn_1/dt = 0$ ,  $n_1(0) = M$ ; this results in the system (with initial condition):

$$\frac{d}{dt} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} 0 \\ s_2 + Ma_{21} \\ \vdots \\ s_m + Ma_{m1} \end{bmatrix}, \quad \begin{bmatrix} n_1(0) \\ n_2(0) \\ \vdots \\ n_m(0) \end{bmatrix} = \begin{bmatrix} M \\ n_2(0) \\ \vdots \\ n_m(0) \end{bmatrix} \quad (10)$$

Note that the mass lost from the system to the compartments which are to be held constant is accounted for, as condition (5) is still satisfied for the diagonal elements of the matrix in equation (10), where the coefficients  $a_{ij}$  are used in the sum.

When more than one of the  $n_i$ 's is constant, this same method can be used. In general, if the  $k$ th compartment/chemical pair is to be constant (say with value  $M_k$ ), then one puts zeros in the  $k$ th row and  $k$ th column, and adds the term  $M_k a_{nk}$  to the  $n$ th row of the source term vector. This is done for every compartment/chemical pair which is to be constant. For example, applied to equation (2), one would obtain the following:

$$\frac{d}{dt} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_{k-1}(t) \\ n_k(t) \\ n_{k+1}(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & a_{22} & a_{23} & \dots & a_{2,k-1} & 0 & a_{2,k+1} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{k-1,2} & a_{k-1,3} & \dots & a_{k-1,k-1} & 0 & a_{k-1,k+1} & \dots & a_{k-1,m} \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & a_{k+1,2} & a_{k+1,3} & \dots & a_{k+1,k-1} & 0 & a_{k+1,k+1} & \dots & a_{k+1,m} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{m2} & a_{m3} & \dots & a_{m,k-1} & 0 & a_{m,k+1} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_{k-1}(t) \\ n_k(t) \\ n_{k+1}(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} 0 \\ s_2 + Ma_{21} + M_k a_{2,k} \\ \vdots \\ s_{k-1} + Ma_{k-1,1} + M_k a_{k-1,k} \\ 0 \\ s_{k+1} + Ma_{k+1,1} + M_k a_{k+1,k} \\ \vdots \\ s_m + Ma_{m1} + M_k a_{m,k} \end{bmatrix}, \quad \begin{bmatrix} n_1(0) \\ n_2(0) \\ \vdots \\ n_{k-1}(0) \\ n_k(0) \\ n_{k+1}(0) \\ \vdots \\ n_m(0) \end{bmatrix} = \begin{bmatrix} M \\ n_2(0) \\ \vdots \\ n_{k-1}(0) \\ M_k \\ n_{k+1}(0) \\ \vdots \\ n_m(0) \end{bmatrix} \quad (11)$$

The method described in this section fits seamlessly into the general process of calculating transition matrices and source terms prior to calling LSODE. In general, one uses all zeros for any row that is to be constant, adds the extra flux terms to the source term vector, and calls LSODE as is done normally.